Beyond stochastic gradient descent for large-scale machine learning

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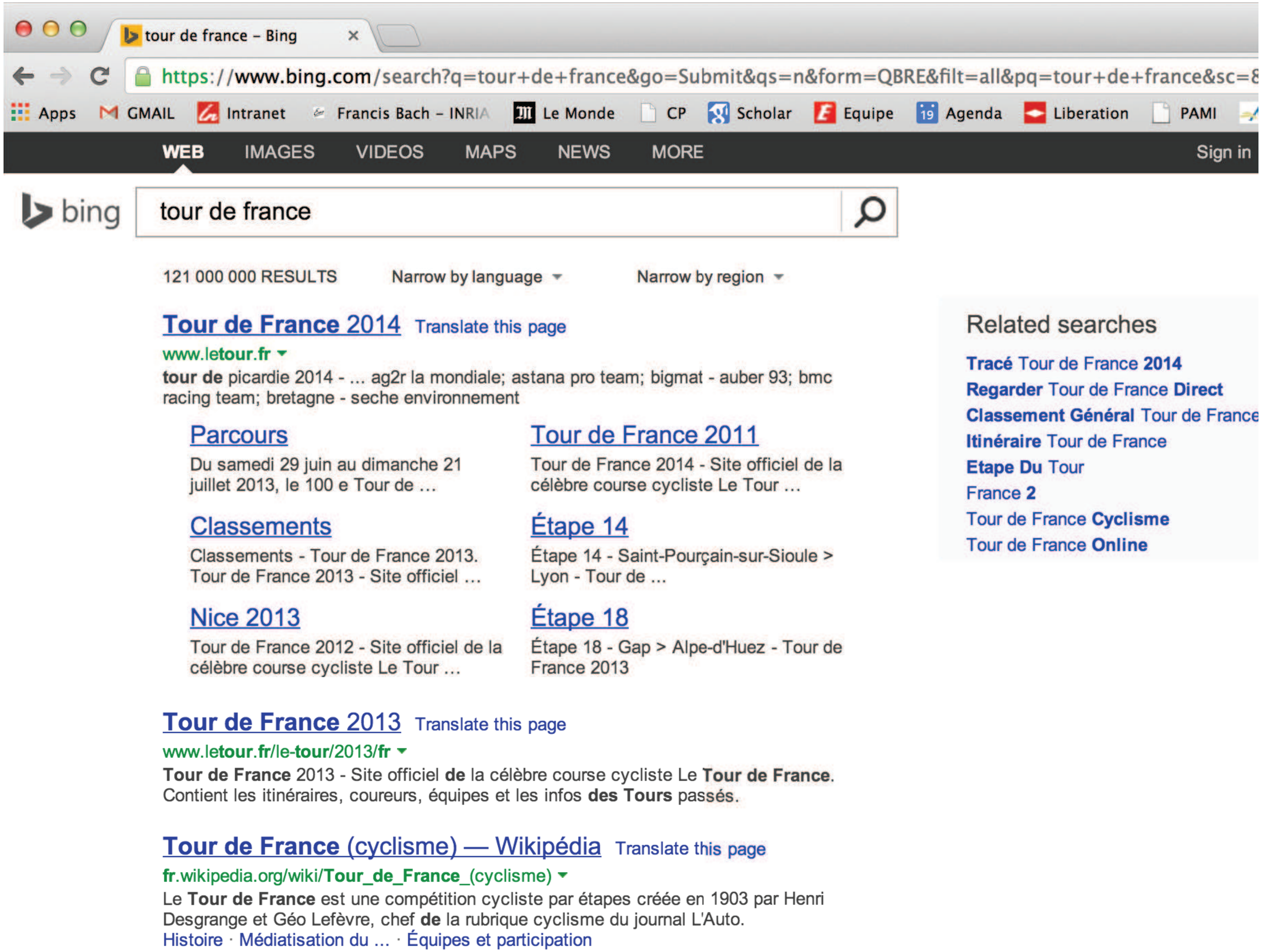
Joint work with Eric Moulines, Nicolas Le Roux and Mark Schmidt - CAP, July 2014

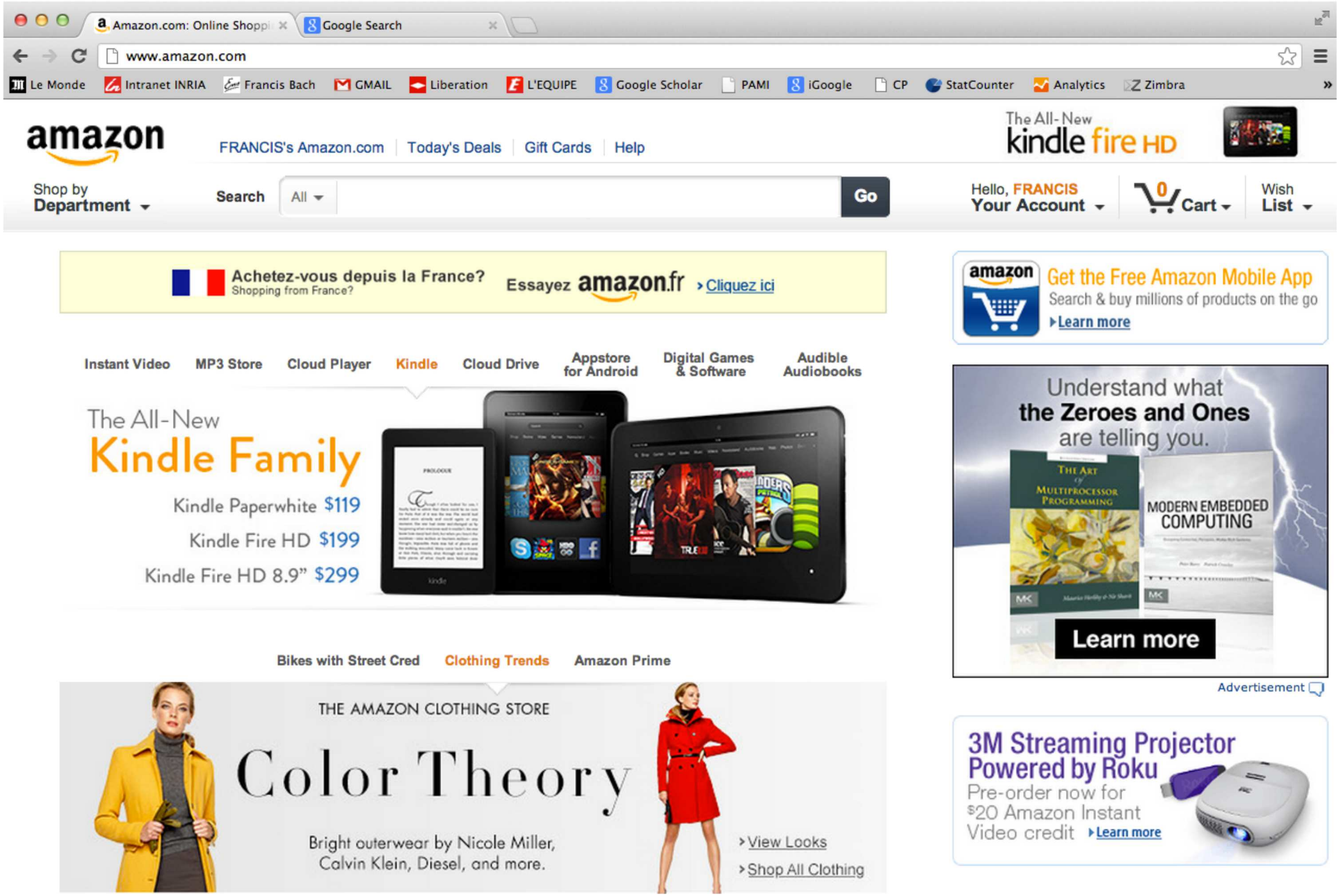
“Big data” revolution?
A new scientific context

- **Data everywhere**: size does not (always) matter
- **Science and industry**
- **Size and variety**
- **Learning from examples**
  - n observations in dimension p

Search engines - Advertising

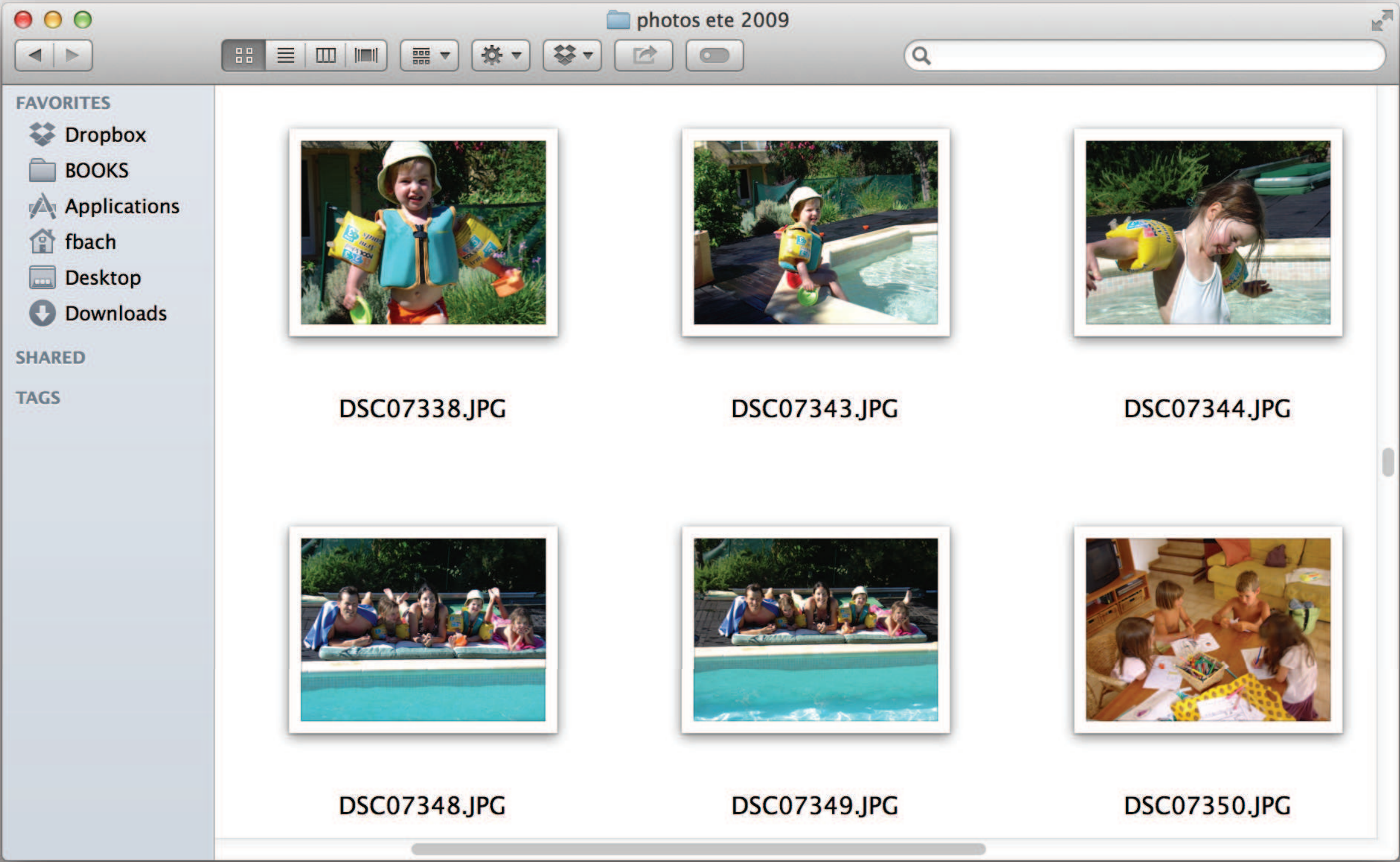


Marketing - Personalized recommendation

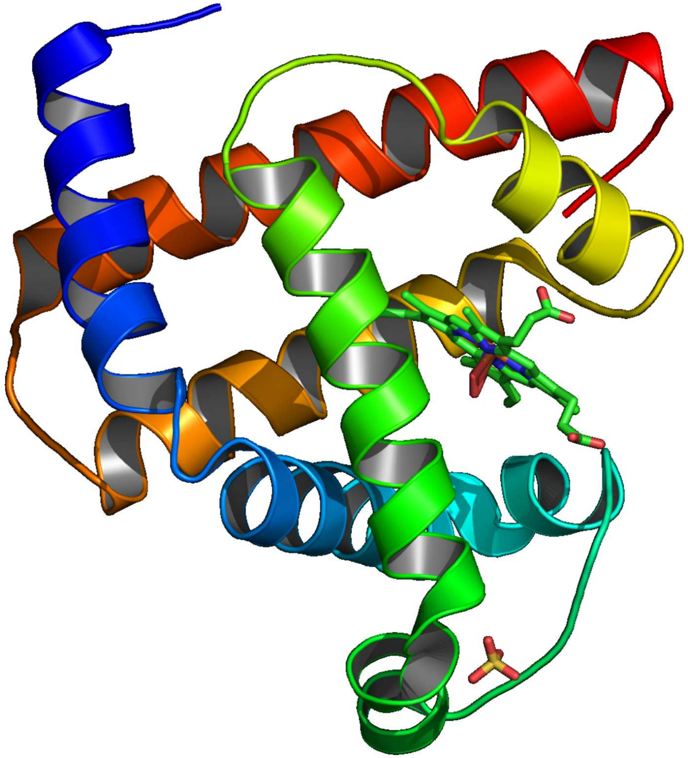


Visual object recognition

Personal photos



Bioinformatics



- **Protein**: Crucial elements of cell life
- **Massive data**: 2 millions for humans
- **Complex data**

Context

Machine learning for "big data"

- **Large-scale machine learning**: **large p, large n**
  - p : dimension of each observation (input)
  - n : number of observations
- **Examples**: computer vision, bioinformatics, advertising

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- **Ideal running-time complexity**: $O(pn)$

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- **Large-scale machine learning**: **large p, large n**
  - p : dimension of each observation (input)
  - n : number of observations
- **Examples**: computer vision, bioinformatics, advertising
- **Ideal running-time complexity**: $O(pn)$
- **Going back to simple methods**
  - Stochastic gradient methods (Robbins and Monro, 1951)
  - Mixing statistics and optimization

Outline

- **Introduction: stochastic approximation algorithms**
  - Supervised machine learning and convex optimization
  - Stochastic gradient and averaging
  - Strongly convex vs. non-strongly convex
- **Fast convergence through smoothness and constant step-sizes**
  - Online Newton steps (Bach and Moulines, 2013)
  - $O(1/n)$ convergence rate for all convex functions
- **More than a single pass through the data**
  - Stochastic average gradient (Le Roux, Schmidt, and Bach, 2012)
  - Linear (exponential) convergence rate for strongly convex functions

Supervised machine learning

- **Data**: n observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$, **i.i.d.**
- Prediction as a linear function $\langle \theta, \Phi(x) \rangle$ of features $\Phi(x) \in \mathbb{R}^p$
- **(regularized) empirical risk minimization**: find $\hat{\theta}$ solution of

$$\min_{\theta \in \mathbb{R}^p} \quad \frac{1}{n} \sum_{i=1}^{n} \ell\big(y_i, \langle \theta, \Phi(x_i) \rangle\big) \quad + \quad \mu \Omega(\theta)$$

convex data fitting term + regularizer

Usual losses

- **Regression**: $y \in \mathbb{R}$, prediction $\hat{y} = \langle \theta, \Phi(x) \rangle$
  - quadratic loss $\frac{1}{2}(y - \hat{y})^2 = \frac{1}{2}(y - \langle \theta, \Phi(x) \rangle)^2$

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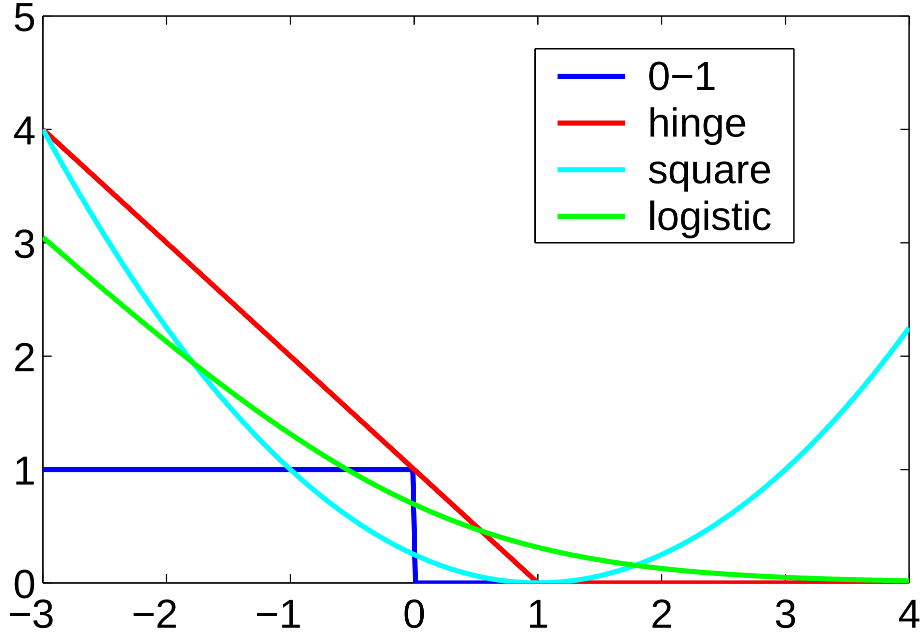
- **Classification** : $y \in \{-1, 1\}$, prediction $\hat{y} = \text{sign}(\langle \theta, \Phi(x) \rangle)$
  - loss of the form $\ell(y \langle \theta, \Phi(x) \rangle)$
  - "True" 0-1 loss: $\ell(y \langle \theta, \Phi(x) \rangle) = 1_{y \langle \theta, \Phi(x) \rangle < 0}$
  - Usual convex losses:



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convex data fitting term + regularizer

- Empirical risk: $\hat{f}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \langle \theta, \Phi(x_i) \rangle)$ training cost
- Expected risk: $f(\theta) = \mathbb{E}_{(x,y)} \ell(y, \langle \theta, \Phi(x) \rangle)$ testing cost
- **Two fundamental questions**: (1) computing $\hat{\theta}$ and (2) analyzing $\hat{\theta}$

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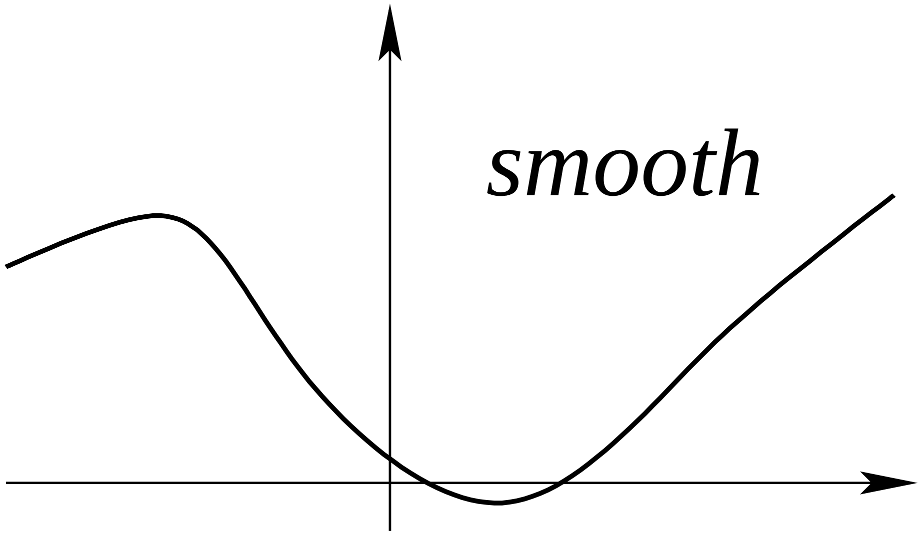
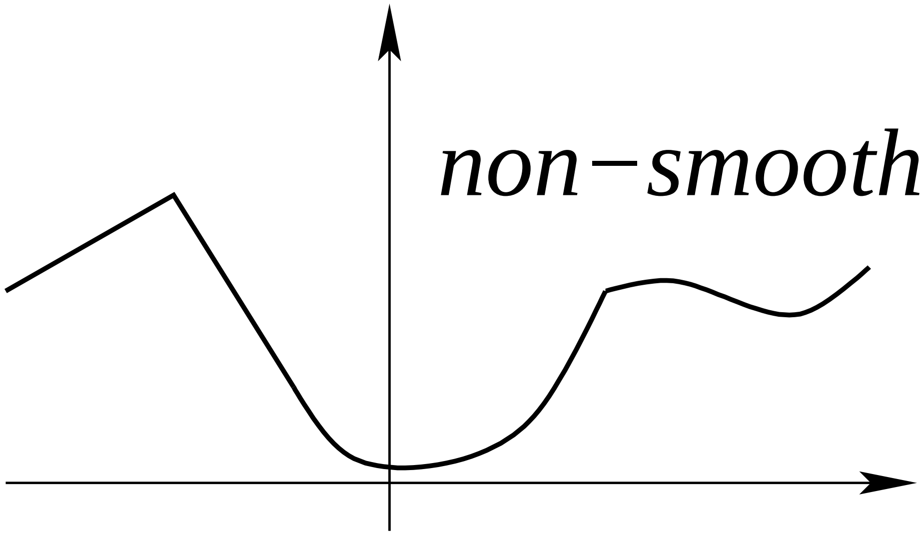
  - **May be tackled simultaneously**

Smoothness and strong convexity

- A function $g : \mathbb{R}^p \to \mathbb{R}$ is L-smooth if and only if it is twice differentiable and

$$\forall \theta \in \mathbb{R}^p, \;\; g''(\theta) \preccurlyeq L \cdot \mathrm{Id}$$





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- **Machine learning**
  - with $g(\theta) = \frac{1}{n}\sum_{i=1}^n \ell(y_i, \langle \theta, \Phi(x_i)\rangle)$
  - Hessian $\approx$ covariance matrix $\frac{1}{n}\sum_{i=1}^n \Phi(x_i) \otimes \Phi(x_i)$
  - Bounded data

Smoothness and strong convexity

- A twice differentiable function $g : \mathbb{R}^p \to \mathbb{R}$ is μ-strongly convex if and only if

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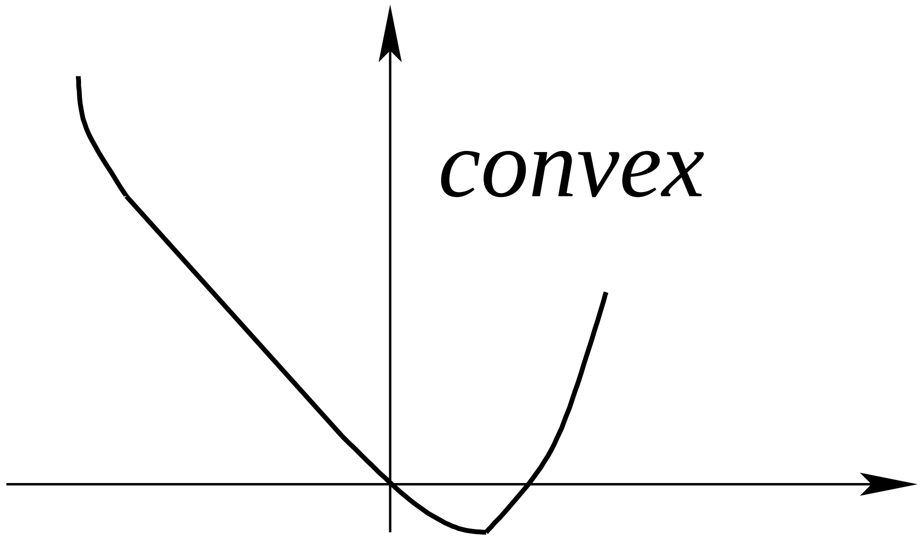

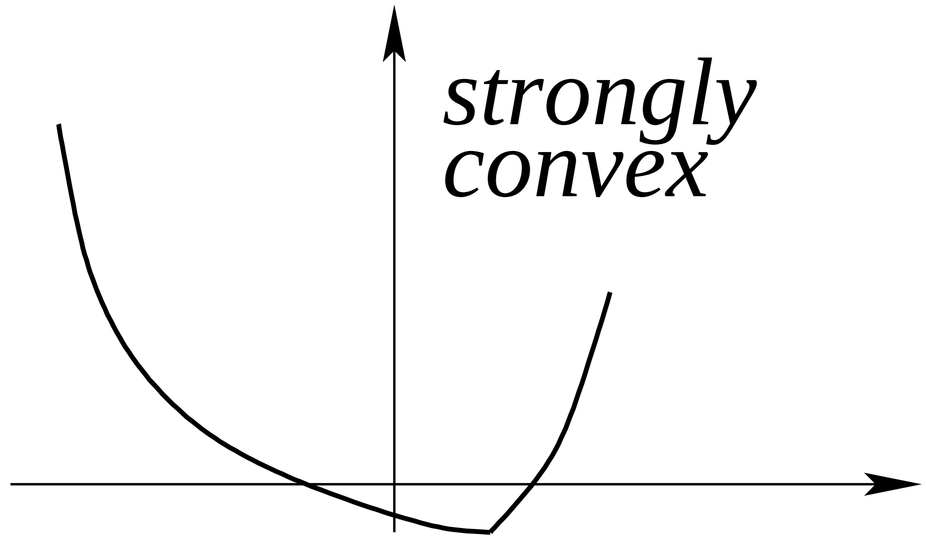

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  - Data with invertible covariance matrix (low correlation/dimension)

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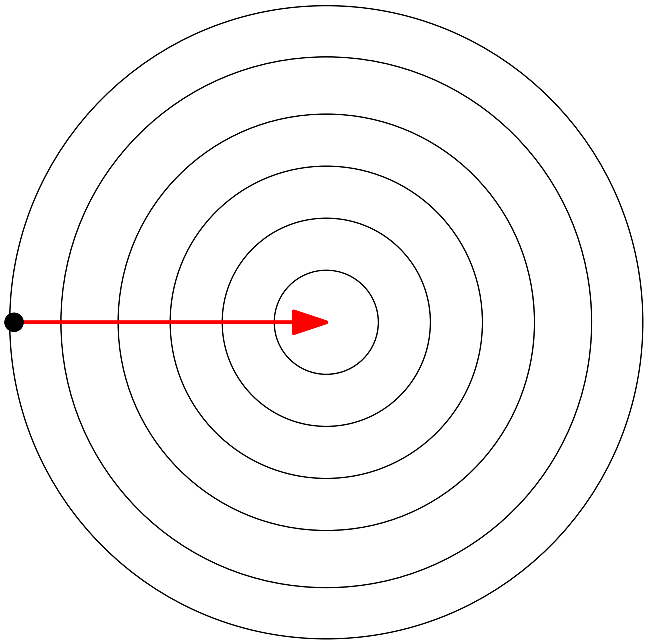
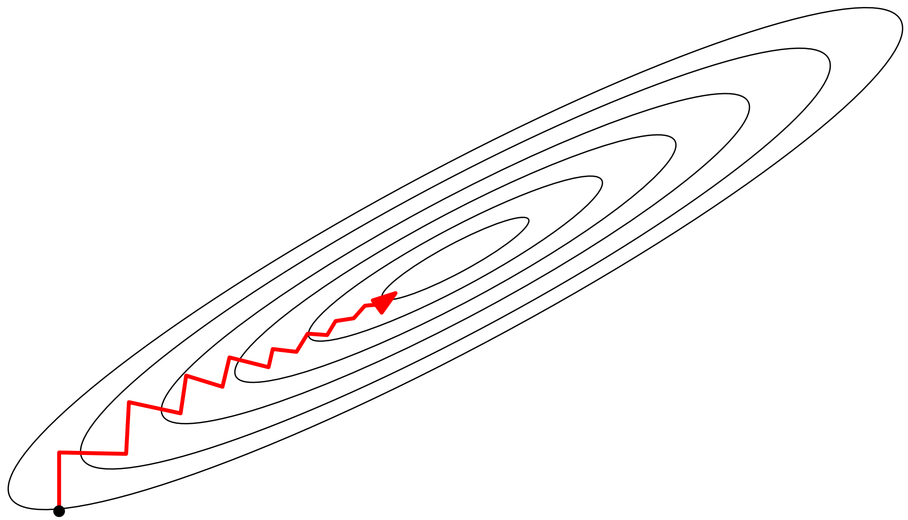
  - Data with invertible covariance matrix (low correlation/dimension)
- **Adding regularization by** $\frac{\mu}{2}\|\theta\|^2$
  - creates additional bias unless μ is small

Iterative methods for minimizing smooth functions

- **Assumption**: g convex and smooth on $\mathbb{R}^p$
- **Gradient descent**: $\theta_t = \theta_{t-1} - \gamma_t \, g'(\theta_{t-1})$
  - $O(1/t)$ convergence rate for convex functions
  - $O(e^{-\rho t})$ convergence rate for strongly convex functions





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- **Newton method**: $\theta_t = \theta_{t-1} - g''(\theta_{t-1})^{-1} g'(\theta_{t-1})$
  - $O\big(e^{-\rho 2^t}\big)$ convergence rate

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- **Key insights from Bottou and Bousquet (2008)**
  1. In machine learning, no need to optimize below statistical error
  2. In machine learning, cost functions are averages

$\Rightarrow$ **Stochastic approximation**

Stochastic approximation

- **Goal**: Minimizing a function f defined on $\mathbb{R}^p$
  - given only unbiased estimates $f'_n(\theta_n)$ of its gradients $f'(\theta_n)$ at certain points $\theta_n \in \mathbb{R}^p$

Stochastic approximation

- **Goal**: Minimizing a function f defined on $\mathbb{R}^p$
  - given only unbiased estimates $f_n'(\theta_n)$ of its gradients $f'(\theta_n)$ at certain points $\theta_n \in \mathbb{R}^p$

- **Machine learning - statistics**
  - $f(\theta) = \mathbb{E} f_n(\theta) = \mathbb{E}\, \ell(y_n, \langle \theta, \Phi(x_n) \rangle) =$ **generalization error**
  - **Loss for a single pair of observations**: $f_n(\theta) = \ell(y_n, \langle \theta, \Phi(x_n) \rangle)$
  - Expected gradient:

$$f'(\theta) = \mathbb{E} f_n'(\theta) = \mathbb{E}\left\{ \ell'(y_n, \langle \theta, \Phi(x_n) \rangle)\, \Phi(x_n) \right\}$$

- Beyond convex optimization: see, e.g., Benveniste et al. (2012)

Convex stochastic approximation

- **Key assumption**: smoothness and/or strong convexity

- **Key algorithm:** stochastic gradient descent (a.k.a. Robbins-Monro)

$$\boxed{\theta_n = \theta_{n-1} - \gamma_n \, f_n'(\theta_{n-1})}$$

  – Polyak-Ruppert averaging: $\bar{\theta}_n = \frac{1}{n+1} \sum_{k=0}^{n} \theta_k$

  – Which learning rate sequence γ_n? Classical setting: $\boxed{\gamma_n = C n^{-\alpha}}$

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- **Running-time** $= O(np)$
  – Single pass through the data
  – One line of code among many

Convex stochastic approximation
Existing work

- **Known global minimax rates of convergence for non-smooth problems** (Nemirovsky and Yudin, 1983; Agarwal et al., 2012)
  - Strongly convex: $O((\mu n)^{-1})$
    Attained by averaged stochastic gradient descent with $\gamma_n \propto (\mu n)^{-1}$
  - Non-strongly convex: $O(n^{-1/2})$
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- **Asymptotic analysis of averaging** (Polyak and Juditsky, 1992; Ruppert, 1988)
  - All step sizes $\gamma_n = Cn^{-\alpha}$ with $\alpha \in (1/2, 1)$ lead to $O(n^{-1})$ for smooth strongly convex problems

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- **A single algorithm for smooth problems with convergence rate $O(1/n)$ in all situations?**

Least-mean-square algorithm

- **Least-squares**: $f(\theta) = \frac{1}{2}\mathbb{E}\big[(y_n - \langle \Phi(x_n), \theta \rangle)^2\big]$ with $\theta \in \mathbb{R}^p$
  - SGD $=$ least-mean-square algorithm (see, e.g., Macchi, 1995)
  - usually studied without averaging and decreasing step-sizes
  - with strong convexity assumption $\mathbb{E}\big[\Phi(x_n) \otimes \Phi(x_n)\big] = H \succcurlyeq \mu \cdot \mathrm{Id}$

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- **New analysis for averaging and constant step-size** $\gamma = 1/(4R^2)$
  - Assume $\|\Phi(x_n)\| \leqslant R$ and $|y_n - \langle \Phi(x_n), \theta_* \rangle| \leqslant \sigma$ almost surely
  - No assumption regarding lowest eigenvalues of H
  - Main result: $\boxed{\mathbb{E} f(\bar{\theta}_{n-1}) - f(\theta_*) \leqslant \dfrac{4\sigma^2 p}{n} + \dfrac{4R^2\|\theta_0 - \theta_*\|^2}{n}}$

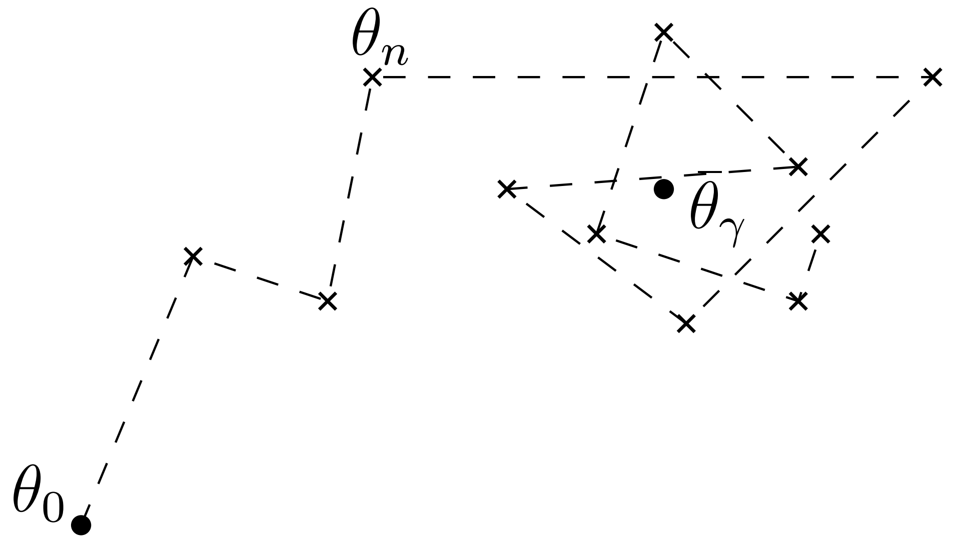
- **Matches statistical lower bound** (Tsybakov, 2003)
  - Non-asymptotic robust version of Györfi and Walk (1996)

Markov chain interpretation of constant step sizes

- LMS recursion for $f_n(\theta) = \frac{1}{2}\big(y_n - \langle \Phi(x_n), \theta\rangle\big)^2$

$$\theta_n = \theta_{n-1} - \gamma\big(\langle \Phi(x_n), \theta_{n-1}\rangle - y_n\big)\Phi(x_n)$$

- The sequence $(\theta_n)_n$ is a homogeneous Markov chain
  - convergence to a stationary distribution π_γ
  - with expectation $\bar{\theta}_\gamma \stackrel{\text{def}}{=} \int \theta \pi_\gamma(\mathrm{d}\theta)$



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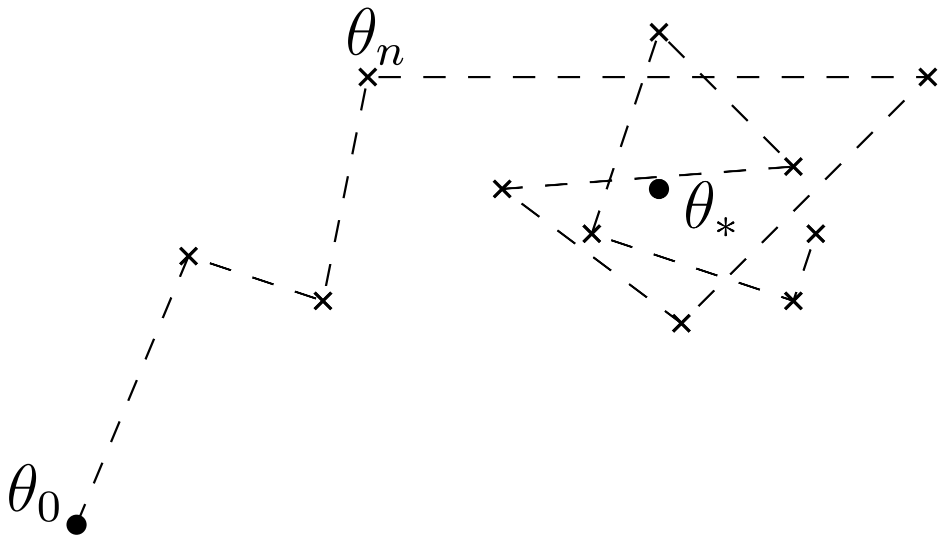
- **For least-squares, $\bar{\theta}_\gamma = \theta_*$**



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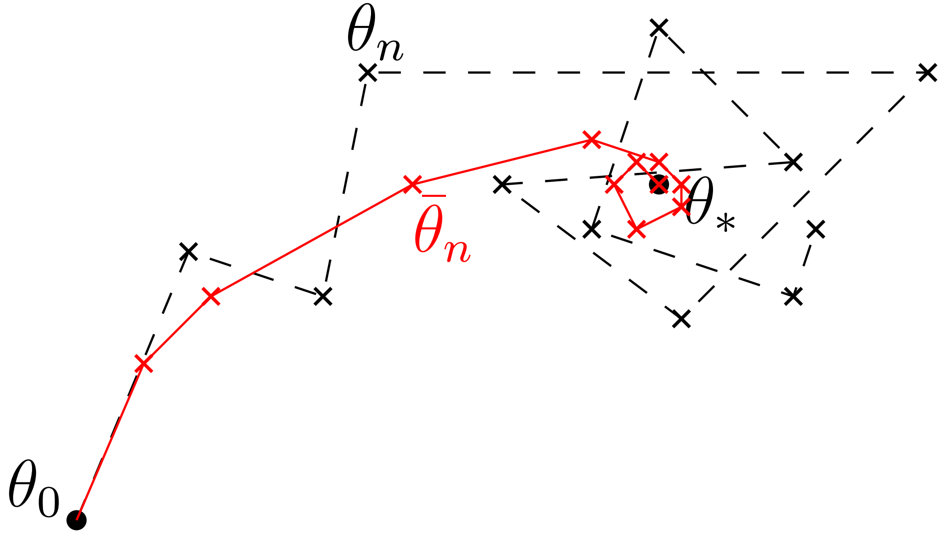

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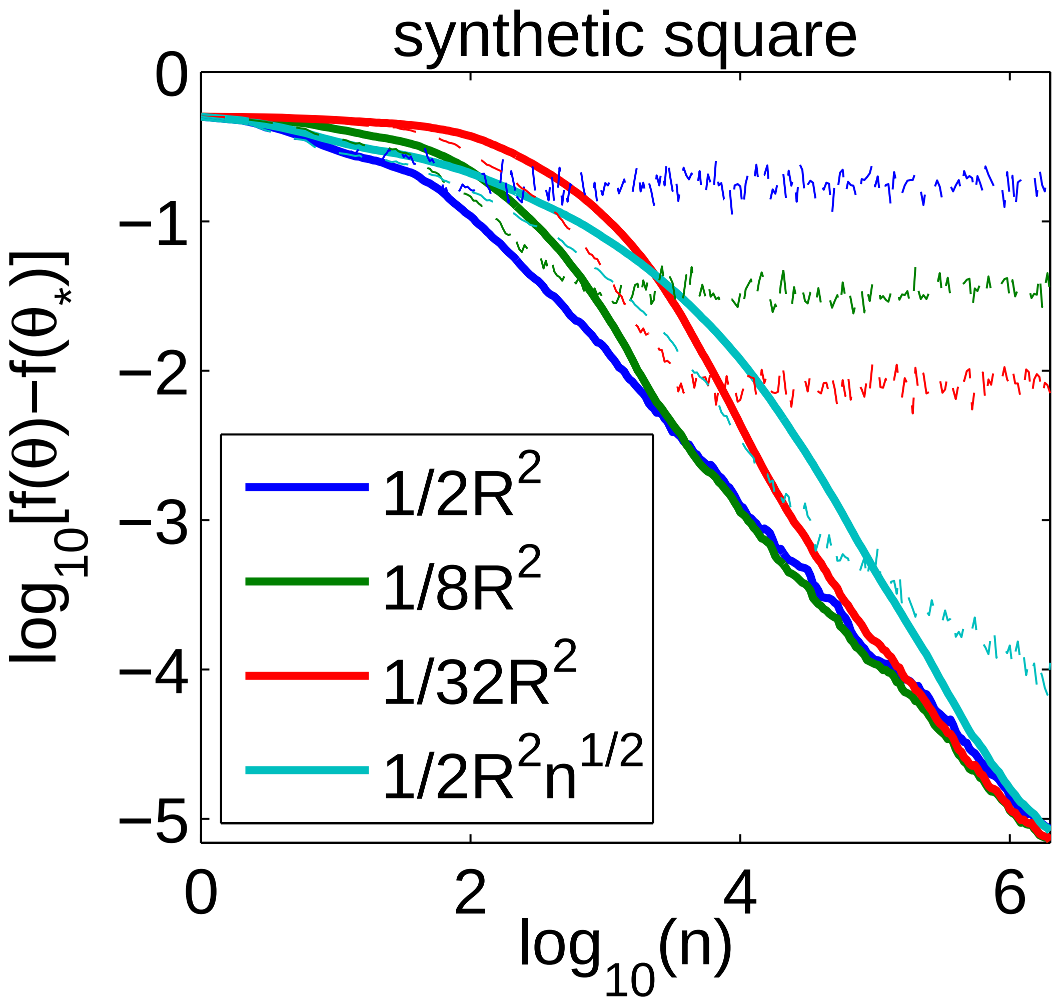
- **For least-squares, $\bar{\theta}_\gamma = \theta_*$**
  - θ_n does not converge to θ_* but oscillates around it
  - oscillations of order $\sqrt{\gamma}$

- **Ergodic theorem:**
  - Averaged iterates converge to $\bar{\theta}_\gamma = \theta_*$ at rate $O(1/n)$

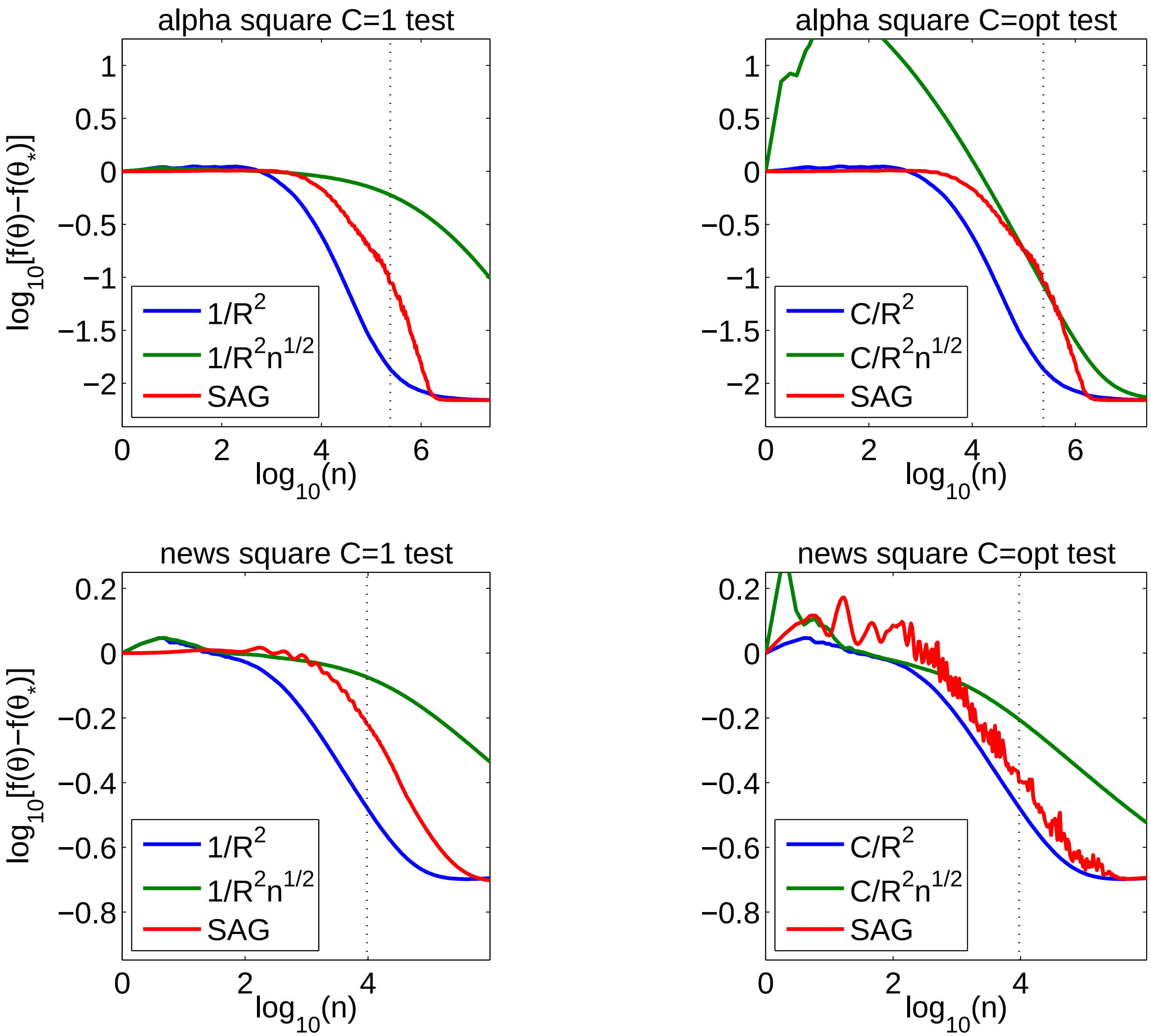
Simulations - synthetic examples

- Gaussian distributions - $p = 20$



Simulations - benchmarks

- *alpha* $(p = 500,\ n = 500\ 000)$, *news* $(p = 1\ 300\ 000,\ n = 20\ 000)$



Beyond least-squares - Markov chain interpretation

- Recursion $\theta_n = \theta_{n-1} - \gamma f_n'(\theta_{n-1})$ also defines a Markov chain
  - Stationary distribution π_γ such that $\int f'(\theta)\pi_\gamma(\mathrm{d}\theta) = 0$
  - When f' is not linear, $f'(\int \theta \pi_\gamma(\mathrm{d}\theta)) \neq \int f'(\theta)\pi_\gamma(\mathrm{d}\theta) = 0$

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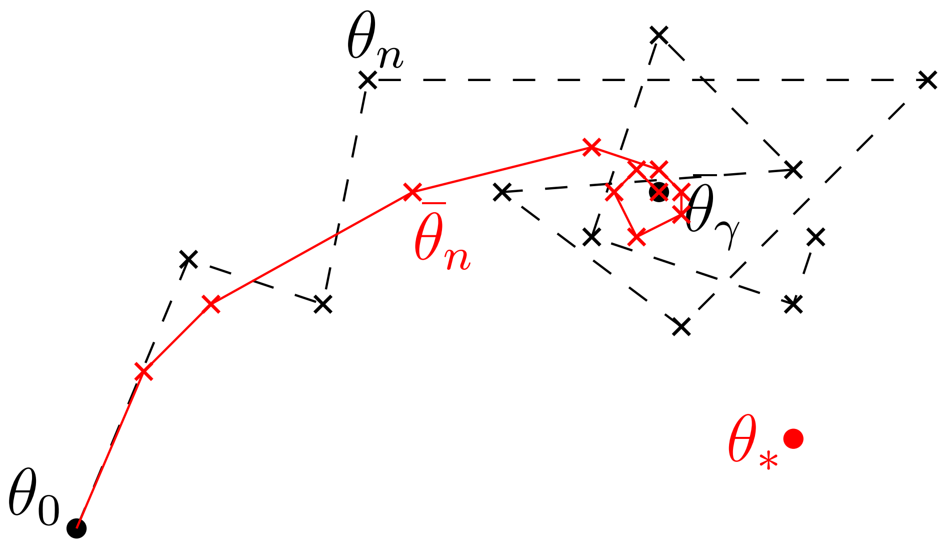
- **θ_n oscillates around the wrong value $\bar{\theta}_\gamma \neq \theta_*$**



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  - Stationary distribution π_γ such that $\int f'(\theta)\pi_\gamma(d\theta) = 0$
  - When f' is not linear, $f'(\int \theta \pi_\gamma(d\theta)) \neq \int f'(\theta)\pi_\gamma(d\theta) = 0$

- θ_n **oscillates around the wrong value** $\bar{\theta}_\gamma \neq \theta_*$
  - moreover, $\|\theta_* - \theta_n\| = O_p(\sqrt{\gamma})$

- **Ergodic theorem**
  - averaged iterates converge to $\bar{\theta}_\gamma \neq \theta_*$ at rate $O(1/n)$
  - moreover, $\|\theta_* - \bar{\theta}_\gamma\| = O(\gamma)$ (Bach, 2013)

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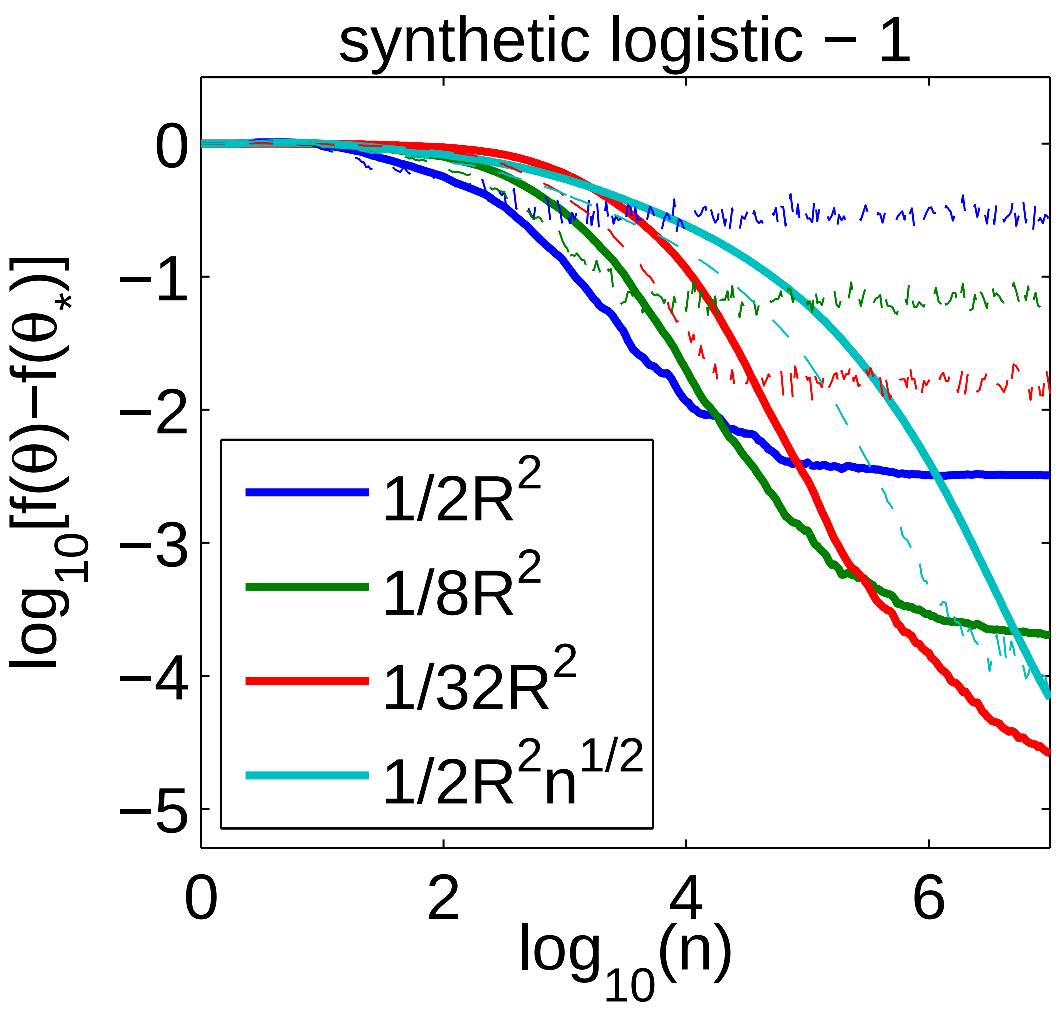

Restoring convergence through online Newton steps

- **Known facts**

1. Averaged SGD with $\gamma_n \propto n^{-1/2}$ leads to *robust* rate $O(n^{-1/2})$ for all convex functions
2. Averaged SGD with γ_n constant leads to *robust* rate $O(n^{-1})$ for all convex *quadratic* functions
3. Newton's method squares the error at each iteration for smooth functions
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Restoring convergence through online Newton steps

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  4. A single step of Newton's method is equivalent to minimizing the quadratic Taylor expansion

- **Online Newton step**

  – Rate: $O((n^{-1/2})^2 + n^{-1}) = O(n^{-1})$
  – Complexity: $O(p)$ per iteration

Restoring convergence through online Newton steps

- The Newton step for $f = \mathbb{E} f_n(\theta) \stackrel{\text{def}}{=} \mathbb{E}\big[\ell(y_n, \langle \theta, \Phi(x_n)\rangle)\big]$ at $\tilde{\theta}$ is equivalent to minimizing the quadratic approximation

$$\begin{aligned} g(\theta) &= f(\tilde{\theta}) + \langle f'(\tilde{\theta}), \theta - \tilde{\theta}\rangle + \tfrac{1}{2}\langle \theta - \tilde{\theta}, f''(\tilde{\theta})(\theta - \tilde{\theta})\rangle \\ &= f(\tilde{\theta}) + \langle \mathbb{E} f_n'(\tilde{\theta}), \theta - \tilde{\theta}\rangle + \tfrac{1}{2}\langle \theta - \tilde{\theta}, \mathbb{E} f_n''(\tilde{\theta})(\theta - \tilde{\theta})\rangle \\ &= \mathbb{E}\Big[f(\tilde{\theta}) + \langle f_n'(\tilde{\theta}), \theta - \tilde{\theta}\rangle + \tfrac{1}{2}\langle \theta - \tilde{\theta}, f_n''(\tilde{\theta})(\theta - \tilde{\theta})\rangle\Big] \end{aligned}$$

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\end{aligned}
$$

- **Complexity of least-mean-square recursion for g is $O(p)$**

$$
\theta_n = \theta_{n-1} - \gamma\big[f_n'(\tilde{\theta}) + f_n''(\tilde{\theta})(\theta_{n-1} - \tilde{\theta})\big]
$$

  - $f_n''(\tilde{\theta}) = \ell''(y_n, \langle \tilde{\theta}, \Phi(x_n)\rangle)\Phi(x_n) \otimes \Phi(x_n)$ has rank one
  - New online Newton step without computing/inverting Hessians

Choice of support point for online Newton step

- **Two-stage procedure**

(1) Run $n/2$ iterations of averaged SGD to obtain $\tilde{\theta}$
(2) Run $n/2$ iterations of averaged constant step-size LMS

  - Reminiscent of one-step estimators (see, e.g., Van der Vaart, 2000)
  - Provable convergence rate of $O(p/n)$ for logistic regression
  - Additional assumptions but no strong convexity

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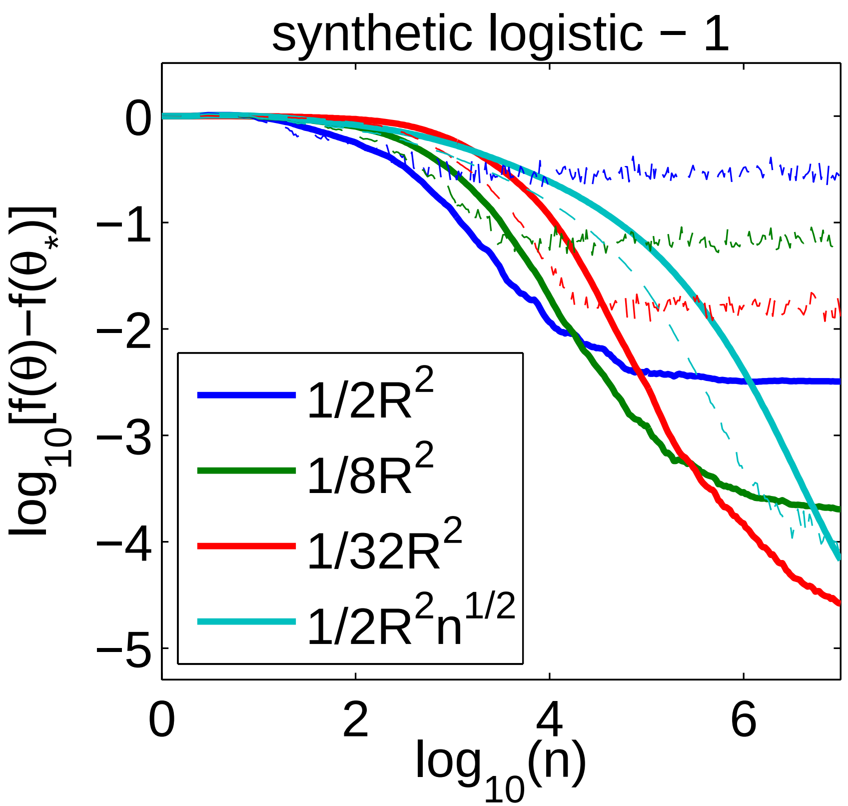
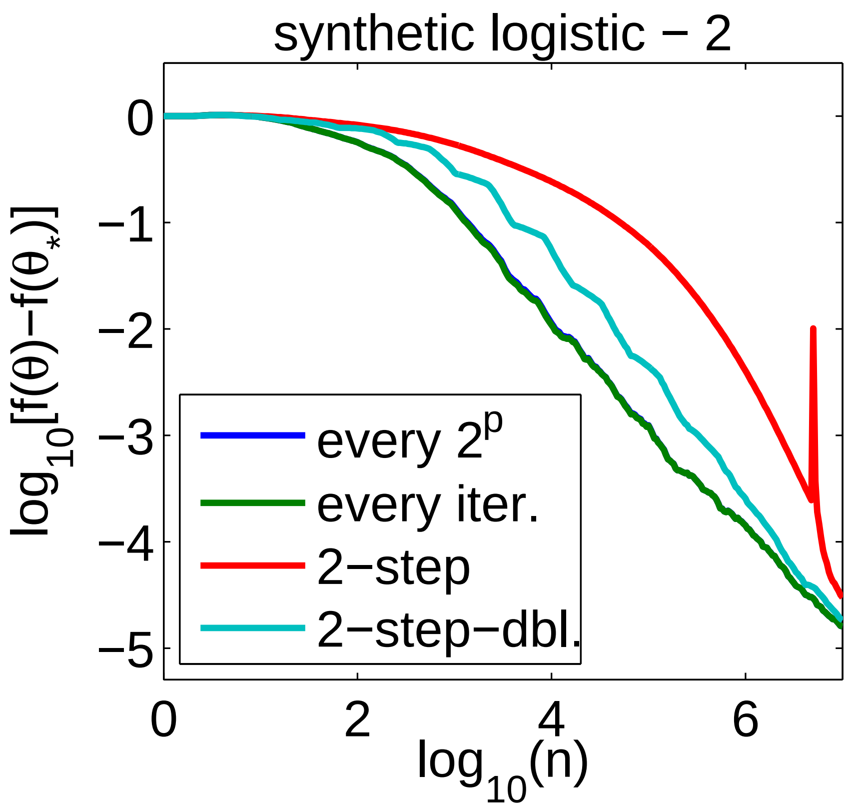
- **Update at each iteration using the current averaged iterate**

- Recursion: $\boxed{\theta_n = \theta_{n-1} - \gamma\big[f'_n(\bar{\theta}_{n-1}) + f''_n(\bar{\theta}_{n-1})(\theta_{n-1} - \bar{\theta}_{n-1})\big]}$
- No provable convergence rate (yet) but best practical behavior
- Note (dis)similarity with regular SGD: $\theta_n = \theta_{n-1} - \gamma f'_n(\theta_{n-1})$

Simulations - synthetic examples

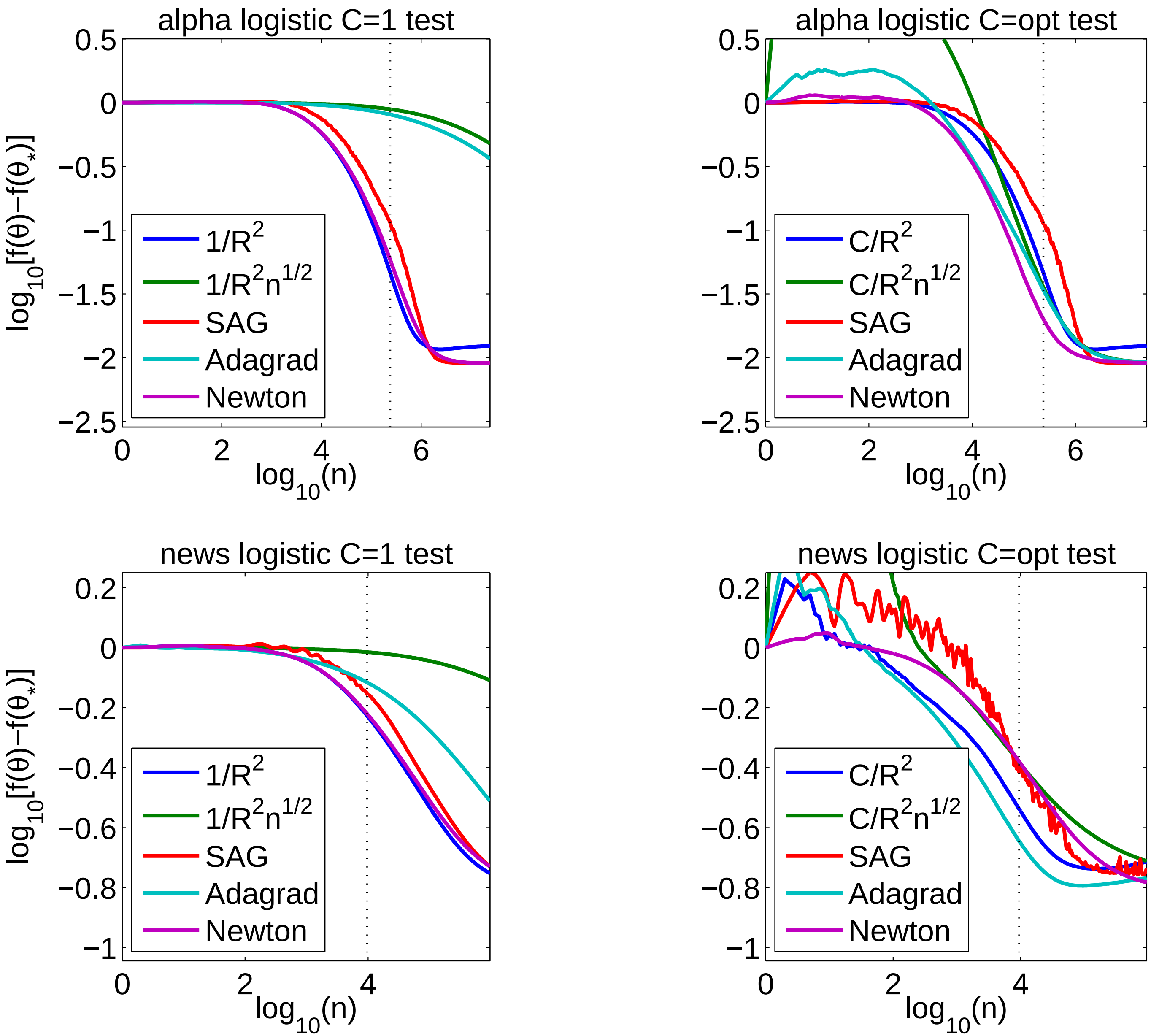
- Gaussian distributions - $p = 20$





Simulations - benchmarks

- *alpha* ($p = 500$, $n = 500\ 000$), *news* ($p = 1\ 300\ 000$, $n = 20\ 000$)



Going beyond a single pass over the data

- **Stochastic approximation**
  - Assumes infinite data stream
  - Observations are used only once
  - Directly minimizes testing cost $\mathbb{E}_{(x,y)}\,\ell(y,\langle\theta,\Phi(x)\rangle)$

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- **Machine learning practice**
  - Finite data set $(x_1, y_1, \dots, x_n, y_n)$
  - Multiple passes
  - Minimizes training cost $\frac{1}{n} \sum_{i=1}^n \ell(y_i, \langle \theta, \Phi(x_i) \rangle)$
  - Need to regularize (e.g., by the ℓ_2-norm) to avoid overfitting

- **Goal**: minimize $g(\theta) = \dfrac{1}{n} \displaystyle\sum_{i=1}^n f_i(\theta)$

Stochastic vs. deterministic methods

- Minimizing $g(\theta) = \frac{1}{n}\sum_{i=1}^{n} f_i(\theta)$ with $f_i(\theta) = \ell\big(y_i, \langle\theta, \Phi(x_i)\rangle\big) + \mu\Omega(\theta)$

- Batch gradient descent: $\theta_t = \theta_{t-1} - \gamma_t g'(\theta_{t-1}) = \theta_{t-1} - \frac{\gamma_t}{n}\sum_{i=1}^{n} f_i'(\theta_{t-1})$

  – Linear (e.g., exponential) convergence rate in $O(e^{-\alpha t})$

  – Iteration complexity is linear in n *(with line search)*

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- Stochastic gradient descent: $\theta_t = \theta_{t-1} - \gamma_t f_{i(t)}'(\theta_{t-1})$
  - Sampling with replacement: $i(t)$ random element of $\{1, \dots, n\}$
  - Convergence rate in $O(1/t)$
  - Iteration complexity is independent of n *(step size selection?)*

Stochastic average gradient (Le Roux, Schmidt, and Bach, 2012)

- **Stochastic average gradient** (SAG) iteration
  - Keep in memory the gradients of all functions f_i, $i = 1, \dots, n$
  - Random selection $i(t) \in \{1, \dots, n\}$ with replacement
  - Iteration: $\theta_t = \theta_{t-1} - \dfrac{\gamma_t}{n} \sum_{i=1}^{n} y_i^t$ with $y_i^t = \begin{cases} f_i'(\theta_{t-1}) & \text{if } i = i(t) \\ y_i^{t-1} & \text{otherwise} \end{cases}$

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- Stochastic version of incremental average gradient (Blatt et al., 2008)

- Extra memory requirement
  - Supervised machine learning
  - If $f_i(\theta) = \ell_i(y_i, \langle \Phi(x_i), \theta \rangle)$, then $f_i'(\theta) = \ell_i'(y_i, \langle \Phi(x_i), \theta \rangle)\, \Phi(x_i)$
  - Only need to store n real numbers

Stochastic average gradient - Convergence analysis

- **Assumptions**
  - Each f_i is L-smooth, $i = 1, \dots, n$
  - $g = \frac{1}{n} \sum_{i=1}^{n} f_i$ is μ-strongly convex (with potentially $\mu = 0$)
  - constant step size $\gamma_t = 1/(16L)$
  - initialization with one pass of averaged SGD

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- **Strongly convex case** (Le Roux et al., 2012, 2013)

$$\mathbb{E}\big[g(\theta_t) - g(\theta_*)\big] \leqslant \Big(\frac{8\sigma^2}{n\mu} + \frac{4L\|\theta_0 - \theta_*\|^2}{n}\Big) \exp\Big(-t \min\Big\{\frac{1}{8n}, \frac{\mu}{16L}\Big\}\Big)$$

  - Linear (exponential) convergence rate with $O(1)$ iteration cost
  - After one pass, reduction of cost by $\exp\Big(-\min\Big\{\frac{1}{8}, \frac{n\mu}{16L}\Big\}\Big)$

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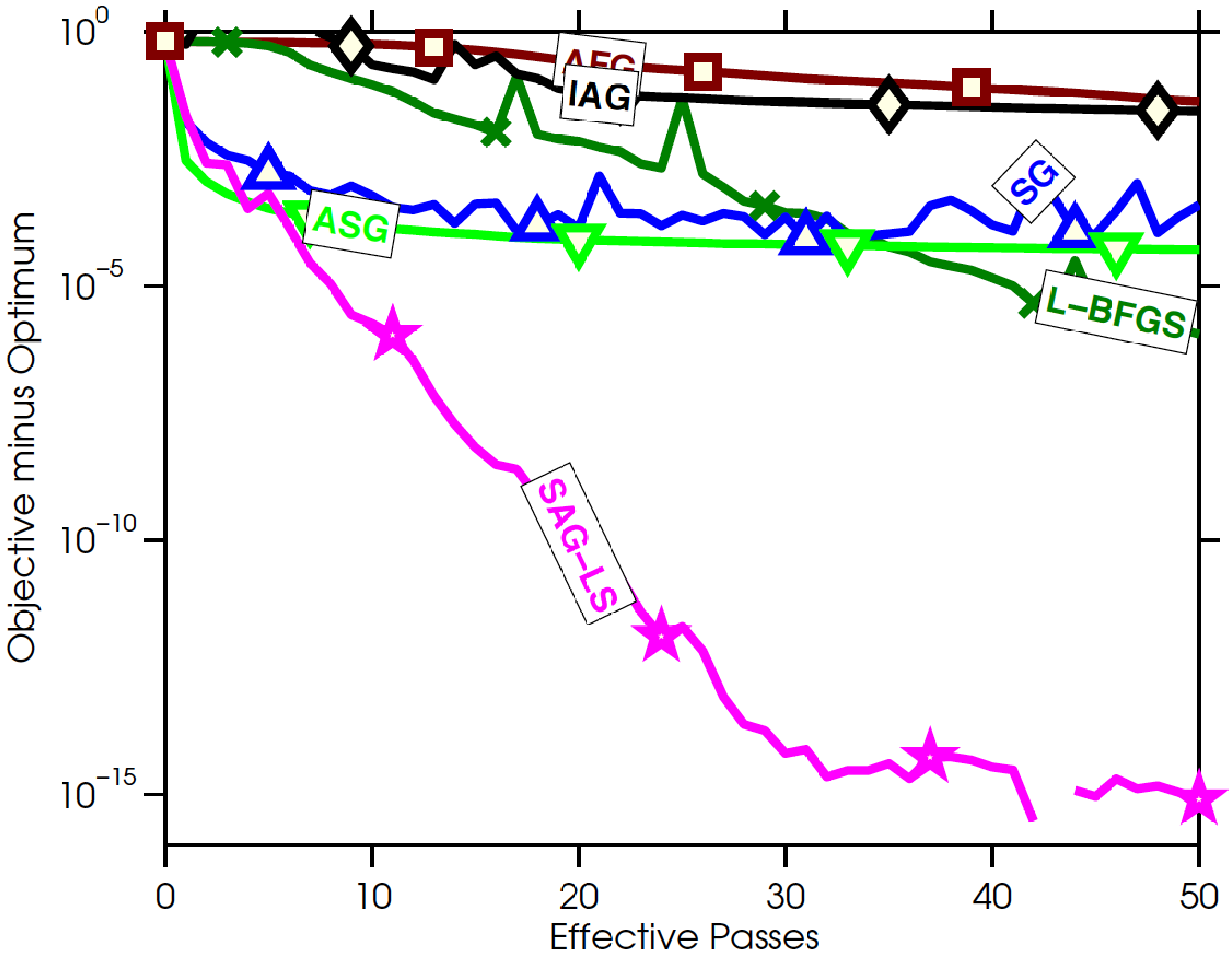
- **Non-strongly convex case** (Le Roux et al., 2013)

$$\mathbb{E}\big[g(\theta_t) - g(\theta_*)\big] \leqslant 48 \frac{\sigma^2 + L\|\theta_0 - \theta_*\|^2}{\sqrt{n}} \, \frac{n}{t}$$

  - Improvement over regular batch and stochastic gradient
  - Adaptivity to potentially hidden strong convexity

spam dataset (n = 92 189, p = 823 470)



Conclusions

- **Constant-step-size averaged stochastic gradient descent**
  - Reaches convergence rate $O(1/n)$ in all regimes
  - Improves on the $O(1/\sqrt{n})$ lower-bound of non-smooth problems
  - Efficient online Newton step for non-quadratic problems
- **Going beyond a single pass through the data**
  - Keep memory of all gradients for finite training sets
  - Randomization leads to easier analysis and faster rates
  - Relationship with Shalev-Shwartz and Zhang (2012); Mairal (2013)
- **Extensions**
  - Non-differentiable terms, kernels, line-search, parallelization, etc.
  - Beyond supervised learning, beyond convex problems

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